Numerical Simulation of Gaseous Microflows by Lattice Boltzmann Method

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Abstract— **This work is concerned with application of the Lattice Boltzmznn Method (LBM) to compute flows in micro-geometries. The choice of using LBM for microflow simulation is a good one owing to the fact that it is based on the Boltzmann equation which is valid for the whole range of the Knudsen number. In this work LBM is applied to simulate the pressure driven microchannel flows and micro lid-driven cavity flows. First, the microchannel flow is studied in some details with the effects of varying the Knudsen number, pressure ratio and Tangential Momemtum Accomodation Coefficient (TMAC). The pressure distribution and other parameters are compared with available experimental and analytical data with good agreement. After having thus established the credibility of the code and the method including boundary conditions, LBM is then used to investigate the micro lid-driven cavity flow. The computations are carried out mainly for the slip regime and the threshold of the transition regime.**

Index Terms— **Microchannel, micro lid-driven cavity, LBM, TMAC, MEMS**

I. INTRODUCTION

Development of Micro-electro-mechanical systems (MEMS) in the recent years has motivated and necessitated the study of flows in micro-scale geometries such as micro lid-driven cavity and micro-channel. Both experimental and computational efforts have been undertaken to understand the specific features of the microscale flows [1-5]. Micro-devices have attracted increasing attention due to their applications in various of fields, such as DNA analysis, cell separation, cell manipulation, biological and chemical analysis [6]. Flows through microchannels are the most common configuration in all of the biomedical applications [7]. Traditional numerical simulations relying on continuum approach and the Navier-Stokes equations break down at higher values of the Knudsen number Kn which equals the ratio of the mean free path of the gas molecules λ to the characteristic length H of the flow system. In the micro-scale geometries Kn is generally high and the Navier-Stokes equation loses validity. It is generally accepted that the Navier-Stokes equations with no-slip boundary conditions are only appropriate when $Kn < 0.001$. For $Kn > 10$ the system can be considered as a free molecular flow. The gas flow for $0.001 < Kn < 0.1$ is termed slip regime and $0.1 < Kn < 10$ is termed transition regime. In the above four regimes, particle based methods such as Molecular Dynamics (MD) and the Direct Simulation Monte Carlo (DSMC) made some progress in simulation of micro-geometries.

However, the computational cost of these methods is usually very large. In the last one and a half decade or so, Lattice Boltzmann method (LBM) has emerged as a new and effective numerical approach of Computational Fluid Dynamics (CFD) and it has achieved considerable success in simulating fluid flows and heat transfer. As opposed to convectional numerical methods based on the discretization of the macroscopic continuum equations, LBM is based on constructing simplified kinetic models containing the physics of microscopic and mesoscopic processes so that averaging can recover macroscopic properties that obeys the continuum equations. The choice of using LBM for microflow simulation is a good one owing to the fact that it is based on the Boltzmann equation which is valid for the whole range of the Knudsen number. In particular, LBM is now being applied to micro-flows in the slip and low-transition regimes. Lattice Boltzmann Methods have earlier been used extensively to simulate incompressible fluid flows with no-slip boundary conditions; but application of LBM to compute gaseous microflows is still an emerging area with some unanswered questions. A few researchers have carried out simulations of the gaseous microflows using Lattice Boltzmann Method. First, Nie et al. [8] used the LBM with bounce-back boundary condition to simulate two-dimensional micro-channel and micro lid-driven cavity flow. They employed the LBM in the no-slip and slip regime, but it is known that the no-slip boundary conditions are generally unrealistic for slip and transition flows and it cannot capture the real microflow characteristics. Tang et al. [10, 11] applied kinetic theory based boundary condition to study gaseous slip flow in micro-scale geometries. Zhang et al. [12] used the tangential momentum accommodation coefficient (TMAC) to describe the gas-surface interactions. Shirani and Jafari [13] applied a combination of bounce-back and specular boundary conditions and their results are in good agreement with the experimental data and analytical solutions. The main objective of the present work is to demonstrate that LBM can be used for flow simulation beyond the continuum regime and that LBM approach could be a valuable alternative approach besides other particle based schemes such as MD and DSMC. Another objective is to examine the effect of varying the Knudsen number, pressure ratio and Tangential Momentum Accommodation Coefficients (TMAC). The paper is organized in four sections. In Section 2 some aspects of the LBM including the Lattice Boltzmann equation and the equilibrium particle distribution functions are presented. Section 3 includes some implementational issues like the lattice model and associated boundary conditions and also the results and discussions. Finally in Section 4 concluding remarks are made.

II. LATTICE BOLTZMANN METHOD

The Lattice Boltzmann equation (LBE) which can be linked to the Boltzmann equation in kinetic theory is formulated as [8]

$$f_i(\mathbf{x}+c_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = \Omega_i \qquad (1)$$

where f_i is the particle distribution function, c_i is the particle velocity along the ith direction and Ω_i is the collision operator. The so-called lattice BGK model with single time relaxation which is a commonly used Lattice Boltzmann method is given by

$$f_i(\mathbf{x}+c_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right) \quad (2)$$

Here $f_i^{(0)}(\mathbf{x},t)$ is the equilibrium distribution function at $\mathbf{x}$,t and τ is the time relaxation parameter. To simulate microscopic gaseous flows, the present LBM relates the relaxation time τ to the Knudsen number from the kinetic theory. Lim et al [9] related with Knudsen number Kn

$$\tau = Kn\,(N_y - 1) \qquad (3)$$

where N_y is the number of lattice nodes in y-direction.

The D2Q9 square lattice used here has nine discrete velocities. A square lattice with unit spacing is used on each node with eight neighbours connected by eight links. Particles residing on a node move to their nearest neighbours along these links in unit time step. The occupation of the rest particle is defined as f_0. The occupation of the particles moving along the axes are defined as f_1, f_2, f_3, f_4, while the occupation of diagonally moving particles are defined as f_5, f_6, f_7, f_8. The particle velocities are defined as

$$
\begin{aligned}
c_i &= 0, \quad i=0 \\
c_i &= (\cos(\pi/4(i-1)), \sin(\pi/4(i-1))), \quad i=1,2,3,4 \\
c_i &= \sqrt{2}(\cos(\pi/4(i-1)), \sin(\pi/4(i-1))), \quad i=5,6,7,8.
\end{aligned}
\qquad (4)
$$

In the nine-velocity square lattice, a suitable equilibrium distribution function has been proposed [9] with,

$$
\begin{aligned}
f_i^{(0)} &= w_i\rho\left[1 - \frac{3}{2}u^2\right], \ i=0 \\
f_i^{(0)} &= w_i\rho\left[1 + 3(c_i.u) + 4.5\,(c_i.u)^2 - 1.5u^2\right], \ i=1,2,3,4 \\
f_i^{(0)} &= w_i\rho\left[1 + 3(c_i.u) + 4.5\,(c_i.u)^2 - 1.5u^2\right], \ i=5,6,7,8
\end{aligned}
\qquad (5)
$$

where the lattice weights are
$w_0 = 4/9, \ w_1 = w_2 = w_3 = w_4 = 1/9, w_5 = w_6 = w_7 = w_8 = 1/36.$
The macroscopic quantities such as density ρ and momentum density ρu are defined as velocity moments of the distribution function f_i as follows:

$$\rho = \sum_{i=0}^{N} f_i, \qquad (6)$$

$$\rho u = \sum_{i=0}^{N} f_i c_i. \qquad (7)$$

III. RESULTS AND DISCUSSION

In this work Lattice Boltzmann Method computation in two micro-geometries, namely, the microchannel and the micro lid-driven cavity are carried out.

A.. Microchannel flow

Lattice Boltzmann Method with D2Q9 model is used to simulate the two-dimensional microchannel flow. The flow is driven by pressure gradient in the main stream direction of flow. The geometry of the microchannel with a flow profile is shown in Figure 1. Initially the *x*-direction velocity is assumed to be uniform through out the channel and *y*-velocity is taken as zero. Density is fixed at a value of 1.0 at inlet. Density is assumed to vary linearly from inlet to outlet, with density constant at each section. Density is fixed at a value of 1.0/PR (PR indicates Pressure ratio) at outlet. Boundary conditions play a crucial role in micro-geometries. For gas flow in microchannels, neither pure no-slip (bounce-back in LBM) boundary condition nor pure free-slip (specular reflection in LBM) can accurately capture the real flow phenomena. In the LBM, the bounce-back boundary condition means that when a particle reaches a wall node, the particle will scatter back to the fluid nodes along its incoming direction, while the specular reflection means the particle will reflect in the specular direction. At the top and bottom walls, combination of bounce-back and specular boundary condition using the tangential momentum accommodation coefficient σ is used to simulate the slip boundary condition in the present work. For gaseous flow in micro-devices the TMAC can be expressed as [12]

$$\sigma = \frac{M_i - M_r}{M_i - M_w} \qquad (8)$$

where M is the tangential momentum of the molecules and the subscripts i, r, w refer to the incident, reflected and wall molecules respectively. Figure 2(a) shows the D2Q9 lattice model, and with respect to Figure 2(b) the boundary conditions at the top wall using TMAC are as follows

$$
\begin{aligned}
f_7 &= \sigma \times f_5 + (1-\sigma) \times f_6 \\
f_4 &= f_2 \\
f_8 &= \sigma \times f_6 + (1-\sigma) \times f_5
\end{aligned}
\qquad (9)
$$

where σ is the TMAC. In case, $\sigma = 0$, the condition will be pure specular that represents pure slip. For $\sigma = 1$, it is pure bounce-back that represents no-slip.

12
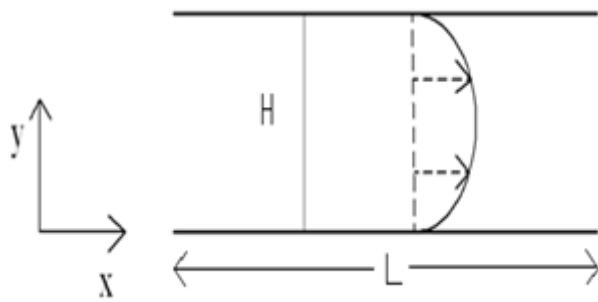
Figure 1. Geometry of microchannel with a flow profile.
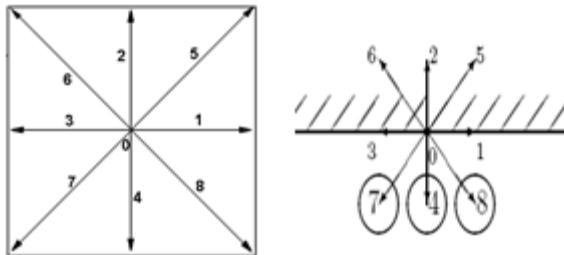
Figure 2. (a) D2Q9 lattice (b) Gas-surface interaction at the top wall
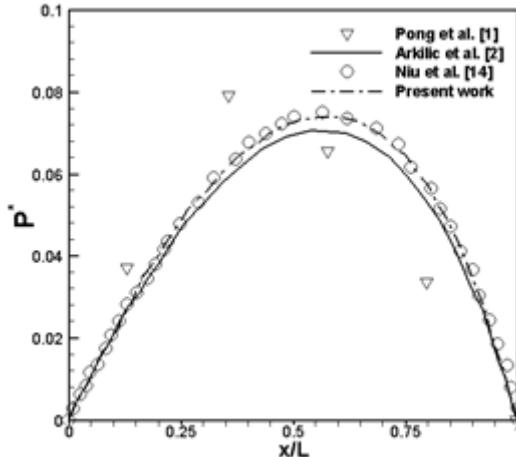
Figure 3. Normalized pressure deviation from the linear pressure distribution ($Kn = 0.053$, PR = 2.02, $\sigma = 0.7$.
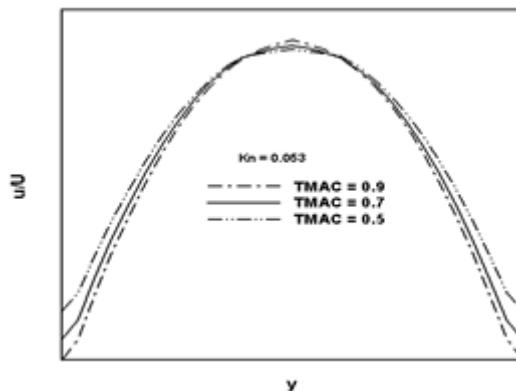

Figure 4. The effect of TMAC on the velocity profile $Kn = 0.053$.
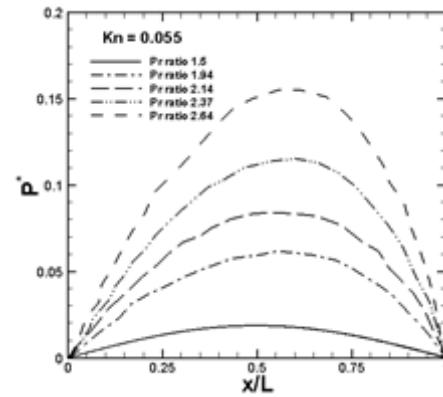
Figure 5. Pressure along the channel for Kn = 0.055.
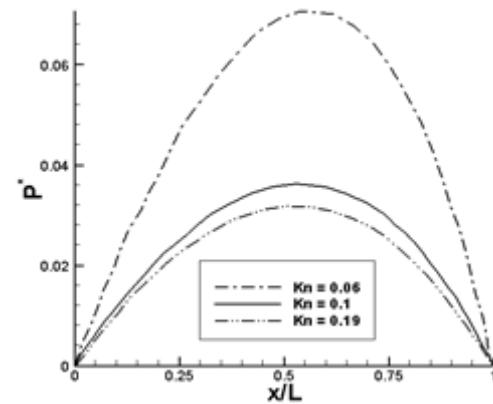
Figure 6. Pressure along the channel for various Kn at $\dfrac{P_{in}}{P_{out}} = 2.0$

All the unknown distribution functions at inlet and outlet are updated by equilibrium distribution functions after finding velocities at inlet and outlet. First, the developed LBM code is used to compute the microchannel flow at a low Knudsen number. The flow with pressure ratio PR = 2.02 and the Knudsen number of 0.053 is studied. Figure 3 shows the normalized pressure deviation from the linear pressure distribution P^* along the microchannel. Established experimental results of Pong et al. [1], analytical results of Arkilic et al. [2] and LBM results of Niu et al. [14] exist for the same problem and these works are used for establishing the credibility of the present LBM code. The pressure distribution result that takes $\sigma = 0.7$ are in reasonable agreement with the experimental and analytical data. Chen et al. [7] indicated that gas flow in microchannels may involve three factors such as compressibility, rarefaction (slip on the surface) and surface roughness effects. That the first two effects are considered in the present work will be shown by our pressure and velocity profile results. The effect of TMAC on the velocity profile at $Kn = 0.053$ is also studied and the results are depicted in Figure 4. As TMAC decreases, slip at the wall increases and the maximum velocity at the centre of the channel decreases.

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13
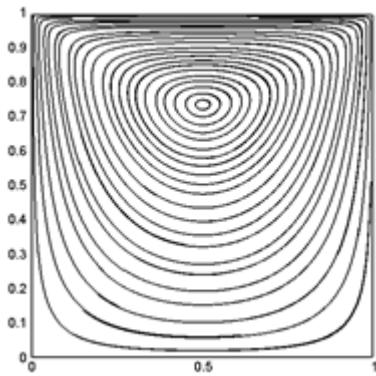
Figure 7. Streamlines at Kn = 0.01, $\sigma = 0.7$.
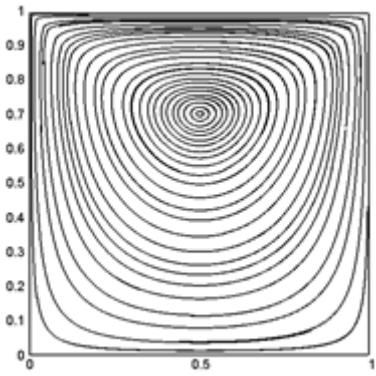
Figure 8. Streamlines at Kn = 0.05, $\sigma = 0.7$.
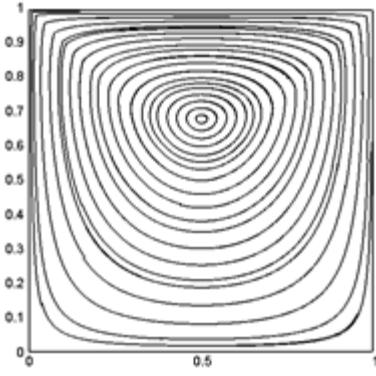
Figure 9. Streamlines at Kn = 0.1, $\sigma = 0.7$.
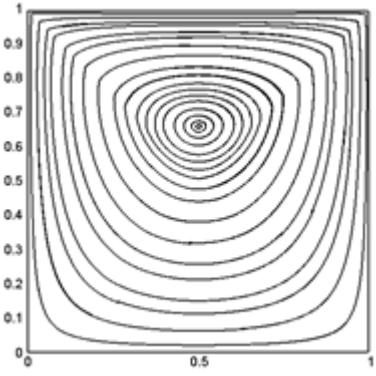
Figure 10. Streamlines at Kn = 0.135, $\sigma = 0.7$.
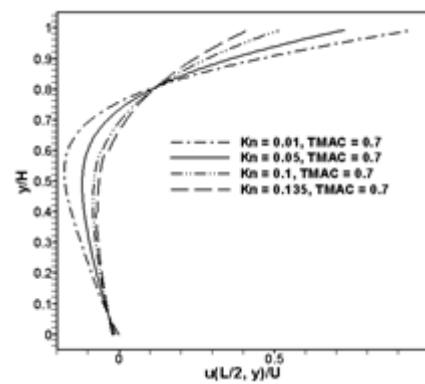
Figure 11. u-velocity profile along the vertical centreline of the cavity for different Knudsen numbers.
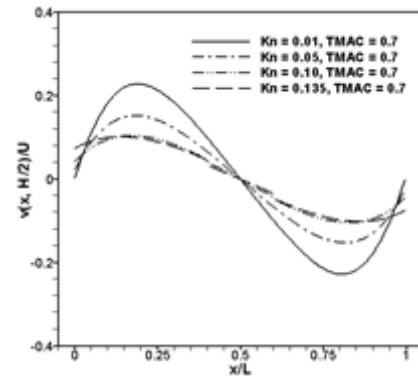
Figure 12. v-velocity profile along the horizontal centreline of the cavity for different Knudsen numbers.

Next the effect of pressure ratio for the same Knudsen number is studied. Pong et al. [1] experimentally investigated the pressure distributions for different Knudsen numbers along the channel, and concluded that they are nonlinear in microchannel flows. Figure 5 shows the nonlinear pressure variation $P^* = \left(P - P_{lin}\right)\big/P_{out}$ for different pressure ratios with $Kn = 0.055$ and $\sigma = 0.7$. Here P_{lin} is the pressure linearly interpolated between the inlet and outlet pressure and P_{out} is the pressure at the exit of the channel. As seen from Figure 5, when the pressure ratio is small the pressure distribution is almost linear. As the pressure ratio increases the pressure distribution become nonlinear due to the compressibility effects. Also seen is the fact that pressure variation peaks shift towards the channel exit as pressure ratio increases. Then, the effect of increasing the Knudsen number is observed. Figure 6 shows the nonlinear pressure variation for different Knudsen numbers for a pressure ratio of 2.0 and . The nonlinearity of the pressure distribution as observed here can be ascribed [7] to the fact that compressibility and rarefaction effects, which are not equal, makes the pressure variation take a different path compared with that for the continuum flow. The results of the present study reveal many interesting features of microchannel flows. It may be concluded that the present study produces results that are in conformity with earlier numerical and experimental observations.

14

B. Micro lid-driven cavity flow

Lattice Boltzmann Method is then used to investigate the micro lid-driven cavity flow. In this problem, the upper wall moves with a constant velocity from the left to right and the other three walls are stationary. The LBM code is used to compute the micro lid-driven flow in a square cavity on a 300×300 lattice. The equilibrium distribution function is then assigned to the particle distribution function at the surface of the moving wall. From our study of the microchannel we observe that $\sigma = 0.7$ produces results that are in good agreement with analytical, experimental and numerical results. That is why on the stationary walls we use a combination of specular and bounce-back boundary condition using a TMAC of . Figures 7, 8, 9 and 10 show the streamline patterns at $Kn = 0.01, 0.05, 0.1$ and 0.135 respectively. With the increase in Knudsen number a slight downward movement of the vortex centre is perceived; however, no horizontal shift of the vortex centre is observed. Figures 11 and 12 show for various Knudsen numbers, the *x*-velocity (*u*) profile along a vertical centreline and the *y*-velocity (*v*) profile along a horizontal centreline passing through the geometric centre of the cavity. The values of *u* at the top and bottom walls (Figure 11) and the values of *v* at the left and right walls (Figure 12) clearly show that slip is nonzero as the flow is not in the continuum regime. The effect of slip is most pronounced at the moving top wall where at the lowest value of $Kn = 0.01$ slip is almost zero and the fluid velocity is almost equal to the lid-velocity so that u is close to 1; for the highest value of $Kn = 0.135$, slip is expectedly maximum and *u* is about 0.5. From Figure 11 one can also observe that the maximum leftward *x*-velocity is obtained for the lowest $Kn = 0.01$. Figure 12 shows that the maximum downward (near the right wall) and maximum upward (near the left wall) *y*-velocity is obtained once again for the lowest $Kn = 0.01$. This is along expected lines as at the lowest *Kn* the ability of the top wall to drive the flow is at its highest and it generates the highest clockwise circulation.

III. CONCLUSION

This work is concerned with application of the LBM to compute flows in two micro-geometries. For the first geometry, namely, the microchannel some experimental, numerical and theoretical results exists, by reproducing which with the LBM an insight about the appropriateness of the present boundary conditions was gained. This knowledge is then utilized when applying the LBM to compute flows in the second geometry, namely, a 2D micro lid-driven cavity. As good care has been taken to include appropriate measures in the computational method, these results enjoy good credibility.

Variation of slip with Knudsen number is studied in some details through the computation of flow in the micro-cavity. It is seen that all the flow features captured are in keeping with the physics of the problem. The Knudsen numbers explored in this work range from the slip to the threshold of the transition regime. To sum up, the present study reveals many interesting features of microchannel and micro lid-driven cavity flows and demonstrates the capability of the LBM to capture this features.

REFERENCES

[1] Kin-Choek Pong, Chih-Ming Ho, Jianqiang Liu, and Yu-chong Tai, "Non-Linear Pressure Distribution in uniform Microchannels," FED-Vol. 197, *ASME winter annual meeting*, pp. 51-56, 1994.

[2] Errol B. Arkilic, Martin A. Schmidt, and Kenneth S. Breuer, "Gaseous Slip Flow in Long Microchannels," *Journal of Microelctromechanical systems*, vol. 6, pp. 167-178, June 1997.

[3] Ali Beskok, George Em Karniadakis, and William Trimmer, "Rarefaction and Compressibility Effects in Gas Microflows," *Transaction of the ASME*, vol. 118, pp. 448–456, 1996.

[4] C. S. Chen, S. M. Lee, and J.D. Sheu, "Numerical Analysis of Gas Flow in Microchannels," *Numerical Heat Transfer Part A*, vol. 33, pp. 749-762, 1998.

[5] Errol B. Arkilic, Kenneth S. Breuer, and Martin A. Schmidt, "Mass flow and tangential momentum accommodation in silicon micromachined channels," *Journal of Fluid Mechanics*, vol. 437, pp. 29-43, 2001.

[6] Mohamed Gad-el-Hak, "The Fluid Mechanics of Microdevices-The Freeman Scholar Lecture," *Journal of Fluids Engineering*, vol. 121, pp. 6-33, March 1999.

[7] A. A. Rostami, A. S. Mujumdar, and N. Saniei, "Flow and heat transfer for gas flowing in microchannels: a review," *Heat and Mass Transfer*, vol. 38, pp. 359–367, 2002.

[8] Xiaobo Nie, Gary D. Doolen, and Shiyi Chen, "Lattice-Boltzmann Simulations of Fluid Flows in MEMS," *Journal of Statistical Physics*, vol. 107, pp. 279-289, 2002.

[9] C. Y. Lim, C. Shu, X. D. Niu, and Y. T. Chew, "Application of the lattice Boltzmann Method to simulate microchannel flows," *Physics of Fluids*, vol. 14, pp. 2209–2308, July 2002.

[10] G. H. Tang, W. Q. Tao, and Y. L. He, "Lattice Boltzmann Method for Simulating Gas Flow in Microchannels," *International Journal of Modern Physics C*, vol. 15, pp. 335-347, 2004.

[11] G. H. Tang, W. Q. Tao, and Y. L. He, "Lattice Boltzmann Method for gaseous microflows using kinetic theory boundary conditions," *Physics of Fluids*, vol. 17, pp. 058101, 2005.

[12] Y. H. Zhang, R. S. Qin, Y. H. Sun, R. W. Barber, and D. R. Emerson, "Gas Flow in Microchannels - A Lattice Boltzmann Method Approach," *Journal of Statistical Physics*, vol. 121, pp. 257-267, 2005.

[13] E. Shirani and S. Safari, "Application of LBM in Simulation of Flow in Simple Micro-Geometries and Micro Porous Media," *African Physical Review*, vol. 1, pp. 0003, 2007.

[14] X. D. Niu, C. Shu, and Y. T. Chew, "Numerical Simulation of Isothermal Micro Flows by Lattice Boltzmann Method and theoretical analysis of the Diffuse scattering boundary condition," *International Journal of Modern Physics C*, vol. 16, pp. 1927–1941, 2005.

[15] Fu-bing Bao, and Jian-zhong Lin, "Burnett Simulations of gas flow in microchannels," *Fluid Dynamics Research*, vol. 40, pp. 679-694, 2008.

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